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The proper representation of particulate phenomena is important for the simulation of many non-ideal particle loaded explosives. These explosives present severe numerical difficulties to simulate because numerical approaches for packed particle beds often behave poorly for the dilute regime and the reverse is often true for methods developed for the dilute regime. This paper presents a multiphase framework for the simulation of these non-ideal explosives that accurately accounts for the particulate behavior in both of these regimes. The capability of this framework is enhanced by the use of prescribed PDF methods for both particle size distributions and the representation of chemical processes. We have validated this framework using several experimental methods that accommodate the separation of momentum flux measurements in two-phase blast flows.

INTRODUCTION

Particle dispersion experiments involving spherical charges provide a useful example of the difficulty of simulating energetically driven particles. The particulate dispersion in Zhang and Frost's experiments are characterized by three distinct regimes: detonics, densely loaded, and dilute flow [1]. After passage of the detonation front, the particles transition from a densely loaded detonation problem to a dilute flow regime within less than five charge radii. The results shown in Figure 1 are for a 11.8 cm diameter nitromethane charge loaded with 0.6 by volume steel spherical particles of diameter, 473 microns. The experimental data are presented as symbols. Three numerical methods are also presented. These methods range from a simple approach to handling multiphase shock-physics, Rusanov and HLL as described by Saurell and Abgrall [2], to the second-order approach used in our framework which is motivated by the work of Chinnayya et al [3]. All of the methods are producing credible simulations. The different methods exhibit different behaviors for the particle phase. Note, a unique feature of the particulate in this charge is that it has sufficient mass to penetrate the explosively driven shock front into the quiescent air. Our approach avoids the primary of defect of most low-order methods, which are overly diffusive. For computational stability reasons, many methods utilize maximum wave speeds that affect adversely the accuracy of the simulation. This is seen in particle fronts that are too slow and air shocks that are excessively damped relative to experiment. This problem is avoided in the second-order approach.

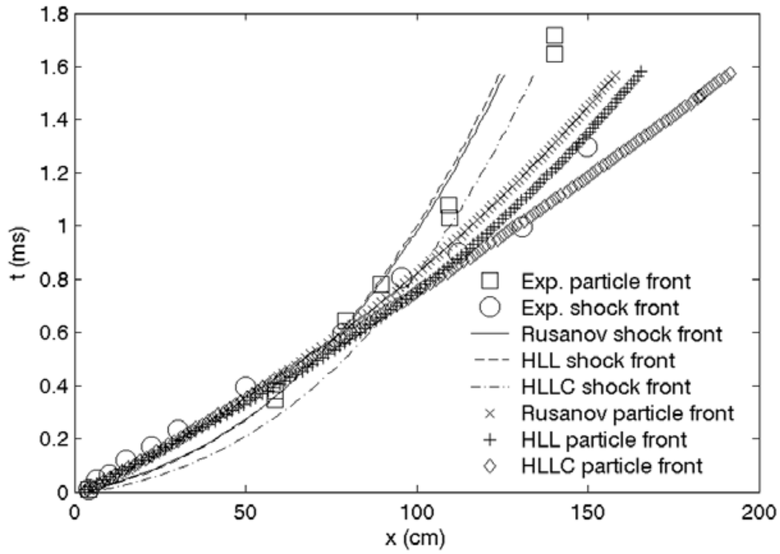

Figure 1. Comparison of experimental and numerical particle and shock front positions [1].

MULTIPHASE FRAMEWORK

The multiphase framework of our work provides an accurate numerical treatment of subgrid effects that often occur in multi-material or multiphase systems. The key aspects of our framework are the second order approach, particle size distributions, and chemical kinetics

Second Order Approach

We utilize an approximate Riemann solver for solving our component contact problems. This approximate solver has been implemented in the context of a traditional MUSCL-Hancock predictor corrector scheme. Typically, a non-conservative formulation is used to predict the needed solution data for the numerical flux at zone faces. This is the predictor. This is then followed by a Riemann solve that computes the numerical fluxes that are used to advance the solution in a second or corrector step. The methodology of the predictor step follows that of Sun and Takayama who define two types of predictors based on approximating a non-conservative formulation of the problem with varying degrees of fidelity [4]. A predictor that was found to be successful was to neglect the off-diagonal and nozzling terms in the predictor. This has the advantage of being second order with respect to advection and substantially improving the accuracy of the material transport. It is computationally very efficient as the same limited slopes can be used throughout.

Particle Size Distributions

Our framework uses the DQMOM approach to model particle size distributions on a subgrid level [5]. This approach accurately models the statistical behavior of a particle distribution via the tracking of only a few moments of the distribution via only a few particle size bins. An example of the application of this method is provided in Figure 2 and is based on the shock driven particle layer of

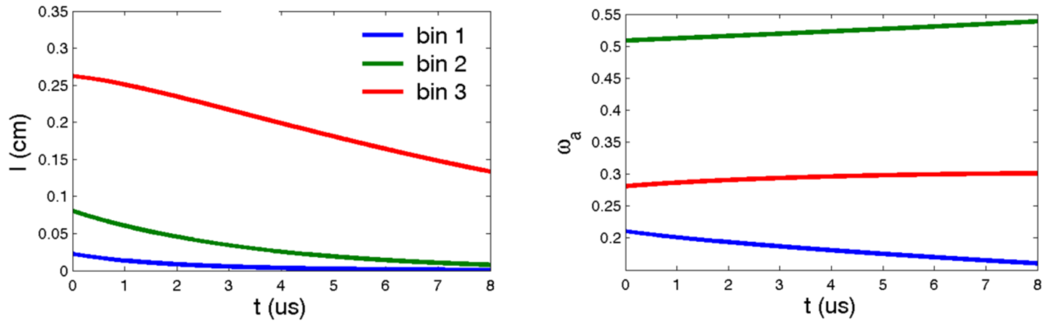

Figure 2. Example of DQMOM approach to model particle size distributions on a subgrid level

Rogue et al.[6]. The particle breakup of the particles after it is initially shocked by a Mach 1.4 air is seen by the decrease in the length scale of each particle bin. Interestingly, and in contrast with more typical particle binning approaches, the weight or mass of the largest particle bin increases as the particle size decreases. A conventional particle model will show mass translating from large to small particle bins. This method by contrast, evolves the moments of the distribution and the particle length scales adjust as this distribution evolves. To preserve the mass or third moment of the distribution, mass can advect from a small size to a large size bin.

Chemical Kinetics

We utilize a coupling of the Cheetah thermochemical code to our multiphase model, Vitello [7]. The use of Cheetah provides a complete characterization of both the initial particle environment composed of a reacting energetic material and the airp roperties needed for the eventual particle dispersion. Cheetah uses rate laws to treat species with the slowest chemical reactions, while assuming other chemical species are in equilibrium. Cheetah supports a wide range of elements and condensed detonation products and can also be applied to gas detonations. Our coupling takes advantage of a sub-grid PDF method for accounting for the effects on non-uniform mixing in augmenting reaction rates. These effects include pre-ignition, extended duration of reactions, and the augmented presence of slow reaction products. A sparse hash table cache of equation of state values is used in Cheetah to enhance the efficiency of kinetic reaction calculations. Cheetah uses MPI communication to manage updates to the cache in large-scale parallel hydrodynamic calculations,.

EXPERIMENTAL METHODS

The focus of our experimental methods has been on quantifying the momentum and energy transport characteristics of the multiphase blast field. This requires the behavior of the gas phase and the solid-phased particulate to be discretely captured in a quantitative manner. Unfortunately, the problem of making separate momentum flux measurements in two-phase blast flows is difficult because of the difference in length scales over which the two phases interact compared to the length scales of typical measurement devices. For this reason, novel approaches are required in order to capture the total momentum and energy flux in two-phase blast flows. We have successfully used the following approaches [8, 9, 10].

Particulate Capture Momentum Trap

The particulate capture momentum method shown in Figure 3 is based on the Held technique for measuring the impulse of objects from explosive blast [11,12]. The addition of a method for capturing and measuring the total flux of the multiphase particulate impacting the object improves on the Held technique. This approach is combined with static pressure gages to allow the separation of the gas phase momentum from the particulate phase momentum. We have also used several geometric shapes (flat plate, sphere, hemisphere, and cone) to provide additional insight into the separation of the gas and particulate phases.

Particulate Streak Recorder

The particle streak recorder shown in Figure 4 is a device that measures the flux of particles in a two-phase blast flow [1, 9, 13]. It does so by employing a spinning drum within a protective shroud. The shroud includes a thin aperture that is aligned toward the oncoming blast and particulate wave. As the two-phase blast wave passes the front of the shroud, the aperture allows a small amount of the particulate and gas products to pass through onto the rotating drum. The rotating drum is designed such that both the particles and the gas phase products are captured on the drum surface. As a result, the drum produces a time history of the particulate that passes through the aperture via the record of particle impacts and gas products across its surface. The angular velocity of the drum is designed so that all of the particulate is captured in less than one revolution. The angular position of the drum is indexed relative to the time of detonation of the explosive. This method has been successfully employed outdoors and in test chambers with standard, inert and rarefied atmospheres.

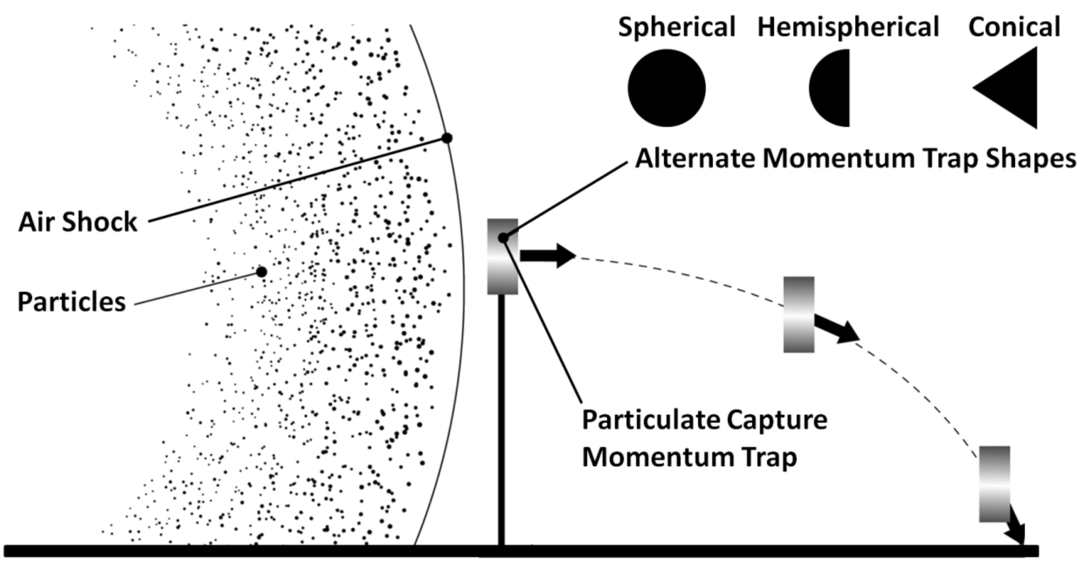

Figure 3. Particulate capture momentum trap

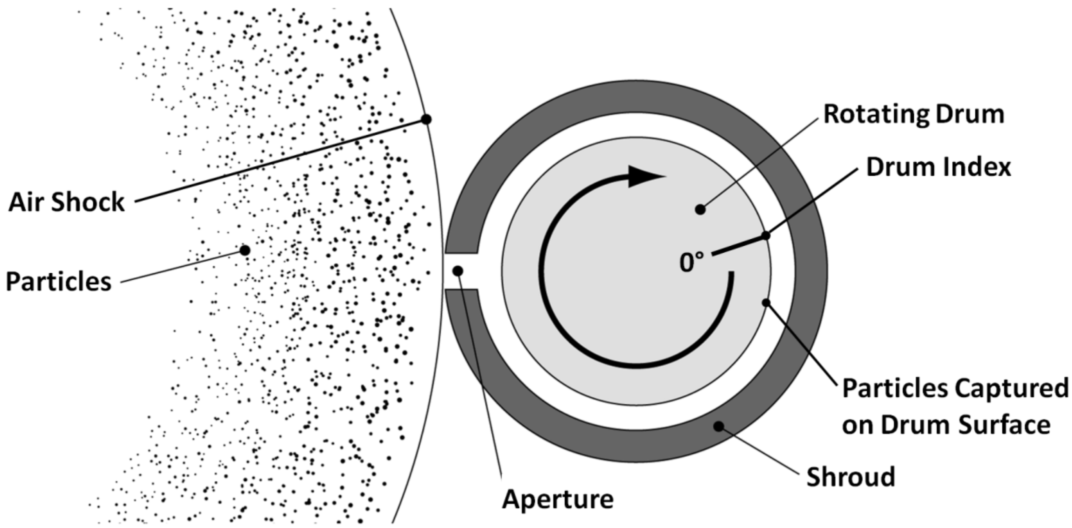

Figure 4. Particle streak recorder.

Blast Bar Gage

The blast bar gage shown in Figure 5 is based on the Hopkinson technique of measuring the stress pulse propagation in a metal bar [14, 15]. The time-resolved pressure history is integrated resulting in an estimate of the impulse per unit area on the face of the bar. As with the particulate capture momentum trap, this method can also use alternate geometric shapes (flat, hemisphere, cone) to provide additional insight into the separation of the gas and particulate phases.

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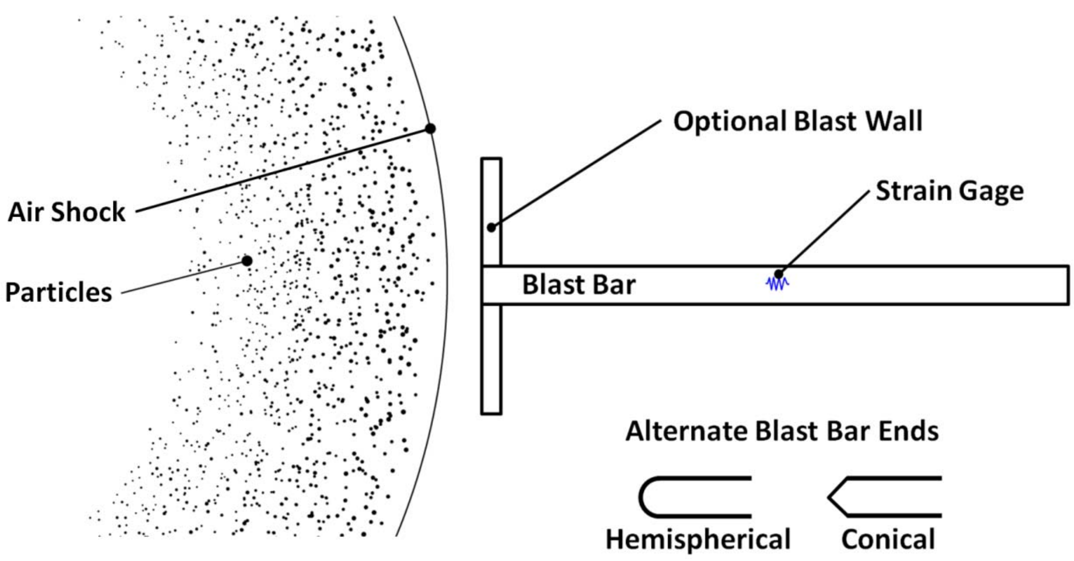

Figure 5. Blast bar gage with optional blast wall and alternate bar ends.

Isolated Particle Method

One of the least understood aspects of energetically driven particles is the coupling of the dense detonics regime to the dilute dispersion regime. We have found that radiography is useful to diagnose the evolution of discrete particles from its initial detonic acceleration to a fluid regime more typical of a blast wave in air. One motivation behind using radiography is its ability to discern between particles and lower density materials such as high explosive and air. Another motivation is the very high temporal resolution obtained by a series of radiographs over other diagnostics.

An example of this methodology is seen by the use of radiography to track the trajectory of particles initially embedded in the mid-plane of a 2-inch diameter by 4-inch high cylinder of high explosive. Embedding the particulate in the midplane of the charge simplifies the geometry of the experiment to a simple cylindrical configuration where the particulate only disperses in the radial and axial directions. Motion out of the midplane can thus be ignored. The radiography uses a rectangular array of 4 X-ray heads and a very large film cassette behind the charge to capture the dispersion of the particles. The experimental configuration is shown in Figure 6. The two initial radiographs make up the left third of the x-ray cassette whereas the final two radiographs take up the bulk of the film on the right.

Some of the most powerful analysis of the particle trajectories arises when we combine them with hydrodynamic modeling using Cheetah for the background air and high explosive products. One of our techniques is to embed the particle trajectories in simulations and to then use the simulation to diagnose properties of the background working fluid. An example of this is shown in Figure 7 where we see the combined analysis product at three positions in time. The ability of the simulated discrete particles to replicate the observed particle dynamics has several important ramifications. Probably the most important of these ramifications is that we can now derive or evaluate advanced particle interaction models that assume semi-analytic solutions for particle-interactions.

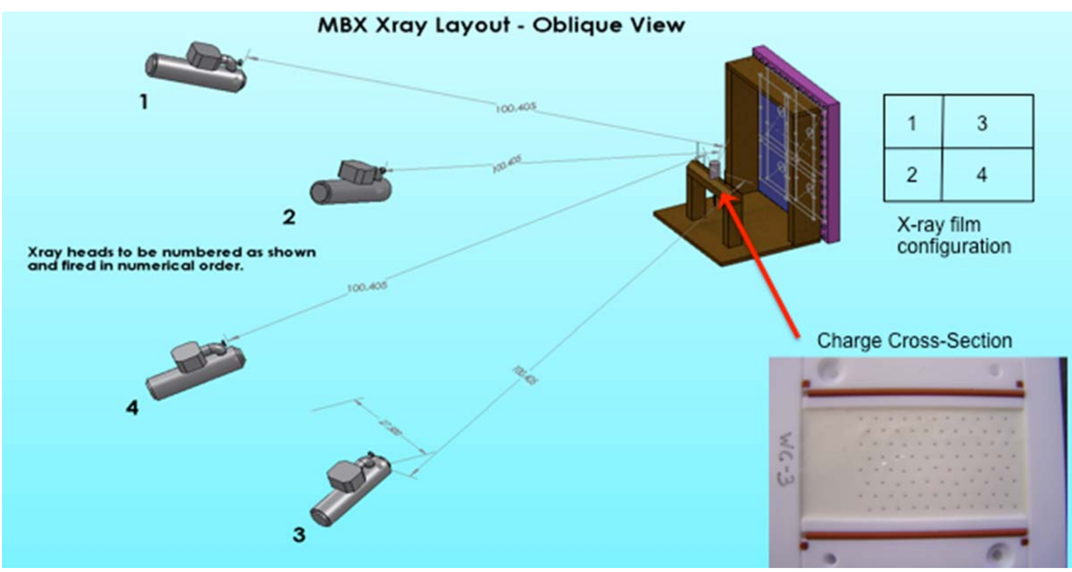

Figure 6. Experiment setup for isolated particle tests

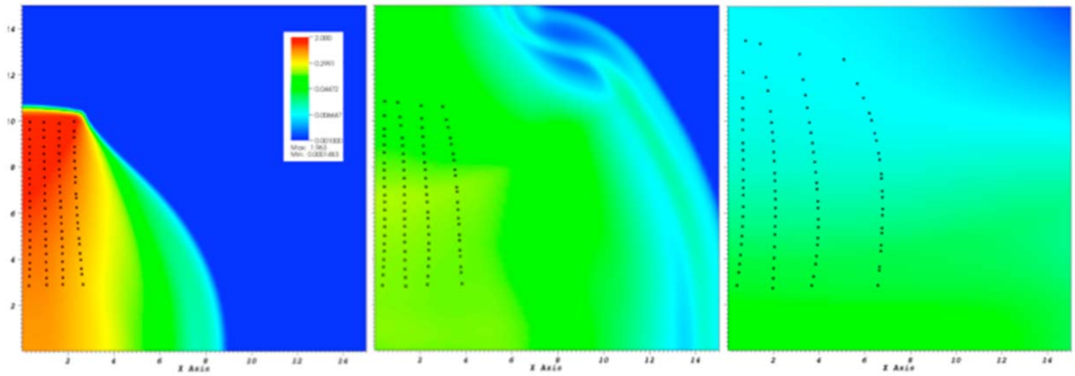

Figure 7. Example of isolated particle trajectories using coupled Cheetah simulations

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